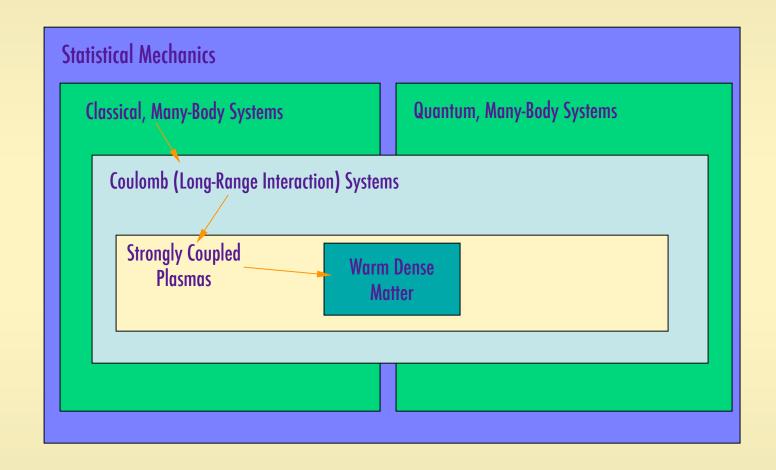
Strongly Coupled Plasmas

Michael S. Murillo Physics Division Los Alamos National Laboratory

- Review of Classical Statistical Mechanics
- Examples of Strongly Coupled Plasmas
- Theoretical and Computational Methods
- A Worked Example: Sedimentation in White Dwarf Interiors
- A Special Case: Warm Dense Matter



Itinerary





Classical Statistical Mechanics Primer

Thermodynamic information (energy, pressure, sound speed, etc.) about a many-body system is obtained from the free energy; here, consider the Helmholtz free energy F(T,V,N).

$$e^{-F/T} = \frac{1}{N!h^{3N}} \int d^{3N}p \, d^{3N}r \, e^{-H/T}$$
 (Note that I use k_B=1.)

The Hamiltonian can be written as:

$$H = \sum_{i} \frac{p_i^2}{2m} + U(\vec{r}_1, ..., \vec{r}_N)$$

The momentum contribution can be integrated exactly, and the remaining portion is the configurational partition function Z.

$$Z = \frac{1}{V^N} \int d^{3N} r \, e^{-U/T}$$

The, in general, the complicated potential energy function U couples all 3N integrals - the classical many-body problem.

Later, Monte Carlo methods will be introduced as a brute-force method to compute these integrals; but, very little physical insight is gained. So, continue with simple analysis methods to understand the essence of the problem.

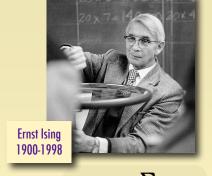


Most Important "Toy Model" - Ising Model

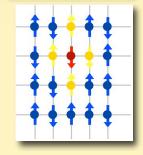
To understand the essence of the many-body problem, let's throw away all complicating issues:

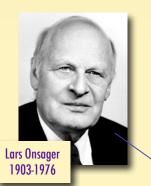
- Don't allow particles to move (easy, since momenta already integrated out)
- Break up space into a simple grid (spatial integrations become sums over grid points)
- Assume very simple interactions (pair, two values)
- Assume minimal nearest neighbor interactions

Such a model is indicative of a spin system that has spin-up and spin-down particles, and was originally formulated in the context of magnetism.



$$H = -J \sum_{\{i, j \to NN\}} s_i s_j$$
$$s_i = \pm 1$$





This greatly simplified model is so rich in physics that:

- effects of dimensionality can be explored (e.g., IM has no phase transition in 1D)
- origin of non-analyticity can be understood
- is isomorphic with many other models (e.g., lattice gas, two level systems, RNA folding, etc.)
- important theoretical methods have been developed with it (e.g., renormalization group)

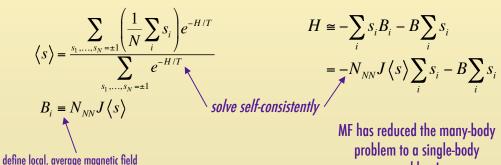
Phase transition in 2D.

Mean Field Solution

Add external magnetic field:

$$H = -J \sum_{\{i,j \to NN\}} s_i s_j - B \sum_i s_i$$
 "single-body" term

Suppose we could calculate the mean spin:

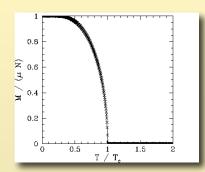


Construct approximate Hamiltonian:

$$H \cong -\sum_{i} s_{i} B_{i} - B \sum_{i} s_{i}$$

$$= -N_{NN} J \langle s \rangle \sum_{i} s_{i} - B \sum_{i} s_{i}$$

MF has reduced the many-body problem to a single-body problem!



When does mean field theory break down?



Systems With Continuous Interactions

Consider an arbitrary classical system's configurational partition function (CPF):

Begin with CPF:
$$Z = \frac{1}{\Omega^N} \int d^{3N} r e^{-U/T}$$

Make mean-field approximation:
$$\approx \frac{1}{\Omega^N} \int d^{3N} r e^{-\sum_i u_i/T}$$

Factorize:
$$= \frac{1}{\Omega^N} \int d^{3N} r \prod_i e^{-u_i/T}$$

Rearrange integrals:
$$= \frac{1}{\mathbf{Q}^N} \int d^3 r_1 e^{-u_1/T} \cdots \int d^3 r_N e^{-u_N/T}$$

Many-body problem is now one-body problem: =
$$\left[\int d^3 r_N e^{-u_N/T}\right]^N$$

The mean-field potential is simply:

$$\begin{split} U &= \frac{1}{2} \int d^3r \, d^3r' n(r) n(r') u(r-r') + \int d^3r \, n(r) u_{ext}(r) \\ &= \int d^3r \, n(r) \left[\frac{1}{2} \int d^3r' n(r') u(r-r') + u_{ext}(r) \right] \\ &\cong \int d^3r \, n(r) \left[\int d^3r' \left\langle n(r') \right\rangle u(r-r') + u_{ext}(r) \right] \end{split}$$

But, what is < n(r) > ?

Finally, we require self-consistency:

$$\langle n(r) \rangle = ne^{-\left(u_{ext}(r) + \int d^3r' \langle n(r) \rangle u_{pair}(r-r')\right)/T}$$

Main Points:

- MFT easily generalized beyond Ising Model to continuous potentials
 - ✓ can expect similarly rich behavior for continuous-potential systems
- Need to solve a non-linear, integral equation to get mean-field solution
 - ✓ such equations are ubiquitous in strongly coupled systems (e.g., HNC approximation)
- ullet Plasma physicists will notice that, when $u_{pair} = u_{Coulomb}$, this is just the Poisson-Boltzmann equation
 - ✓ thus, most of "normal" plasma physics is based on an uncontrolled approximation



When Does Mean-Field Theory Fail?

In general, this is a difficult question to answer, and one needs to resort to formalisms (e.g., field theory, renormalization group) beyond the scope of this lecture. The key physics result is that MFT fails when *fluctuations* become important. In fact, we can use the MFT result to illustrate this; specifically, we can look at Coulomb systems.

First, consider systems with long-range interactions; such systems are pathological!

$$\int d^3r' \left\langle n(r) \right\rangle u_{pair}(r-r')/T \approx \frac{4\pi nC}{T} \int_{R_1}^{R_2} dr \, r^2 \, \frac{1}{r^m} \rightarrow \infty$$

To fix this, introduce a single, discrete particle at the origin and add a neutralizing background of opposite charge - the "One-Component Plasma" model.

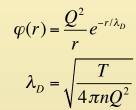
Coulomb systems (plasmas) are special in this regard! Other systems have similar issues; e.g., biological systems with dipole interactions.

$$\langle n(r) \rangle = ne^{-u_{ext}(r)/T - \int d^3r \cdot \langle n(r) \rangle u_{pair}(r-r')/T - u_b/T}$$
$$= ne^{-Q\varphi(r)/T}$$

$$u_{ext}(r) = \frac{Q^2}{r} = u_{pair}(r)$$

$$\nabla^2 \varphi(r) = -4\pi \left[Q\delta(r) + Q\langle n(r) \rangle - Qn \right]$$

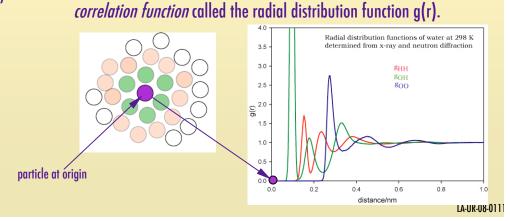
The linear solution can be obtained easily.



In statistical mechanics, this is referred to as the "Yukawa potential".



Peter Debye

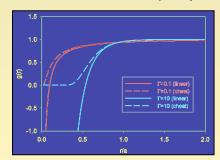


We have implicitly introduced a new type of density - the density given that there is a discrete particle at the origin; in fact, this is a

The Breakdown of Mean-Field Theory Leads to the Concept of Strongly Coupled Plasmas

Most plasma texts are happy to show you the Debye-Hückel (DH) potential, but they rarely show you the density from which it was obtained. Let's look at the density, which is the DH radial distribution function (RDF).

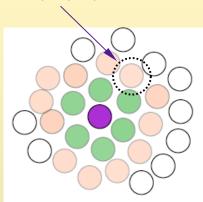
$$\begin{split} \left\langle n(r)\right\rangle &= ne^{-Q\varphi(r)/T} \\ &\approx n\left(1-Q\varphi(r)\,/\,T\right) \qquad \text{Remember, DH is the linear solution.} \\ &= n\!\left(1-\frac{Q^2}{rT}\,e^{-r/\lambda_D}\right) \end{split}$$



Major problem! DH theory predicts a negative density (RDF) at small enough r; clearly, this linear, MFT solution has completely broken down.

In practice, one is not bothered by this failure, if the negative density occurs at distances that are irrelevant to the problem at hand. What if negative density occurs everywhere?

volume occupied by one particle



sphere has radius a - the ion-sphere radius

$$a = \left(\frac{3}{4\pi n}\right)^{1/3}$$
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If we can ignore the exponential, negative density is everywhere when

$$\frac{Q^2}{aT} > 1$$

Thus, complete breakdown of MFT for Coulomb systems can be quantified by the so-called Coulomb coupling parameter

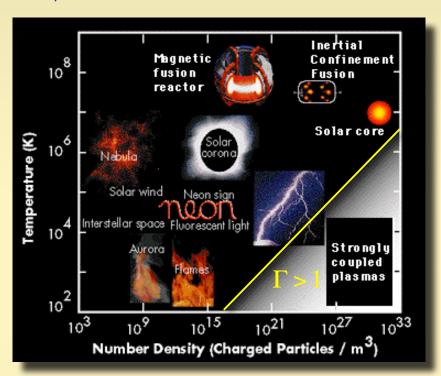
$$\Gamma = \frac{Q^2}{aT} = \frac{\langle \text{potential energy} \rangle}{\langle \text{kinetic energy} \rangle}$$

Main Points:

- Special care must be taken for many-body systems with long-range interactions, such as dipoles and Coulomb systems
- The OCP model has been introduced
- The DH problem has introduced the concept of the RDF
- The DH solution has allowed us to estimate when MFT breaks down
- Failure occurs when we observed the density near a discrete particle
- MFT fails when the Coulomb coupling parameter Γ exceeds unity, which introduces the concept of strongly coupled plasmas

What Are Some Examples Of Real Strongly Coupled Plasmas?

First, let's look at what information is contained with Γ .



There are many examples:

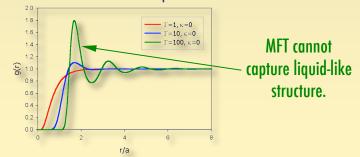
- giant planets
- brown dwarfs
- white dwarfs
- neutron star surfaces
- quark-gluon plasmas
- early-time ICF experiments
- etc.

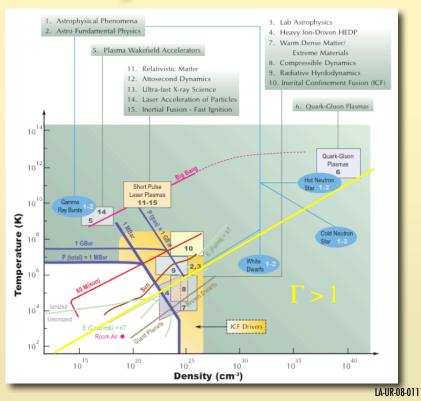
Los Alamos NATIONAL LABORATORY Thus, the statistical mechanics of systems with long-range potentials in which MFT fails is important for many applications.



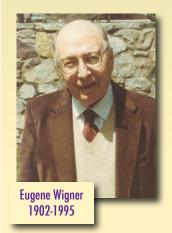
Strong coupling is some combination of:

- high charge
- high density
- low temperature





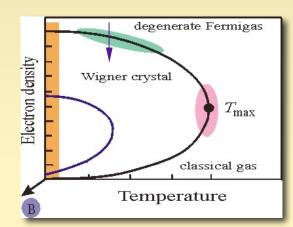
Reduced Dimensionality Systems



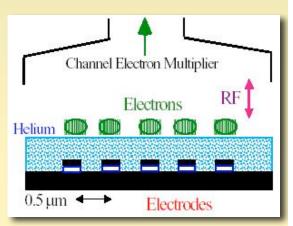
Wigner predicted that *expanded* electron gases would form crystals (BCC in 3D).

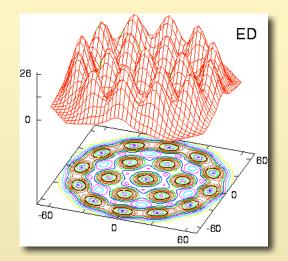
This is non-trivial: the usual solids we think of crystallize because of bonding (attractive interactions).

Experiments tend to be easier in 1D and 2D.



Electrons on Liquid Helium





This field is too large to cover here:

- 1D traps
- electrons trapped in semiconductor junctions
- quantum computing
- nanowires
- clusters
- bilayers
- etc.

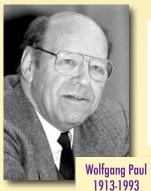


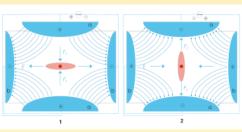
Non-Neutral and Neutral Ultra-Cold Plasmas

Laser-cooling technology now allows us to cool ions and atoms to ultra-cold temperature with T $<\mu$ K.

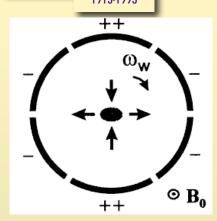
Non-Neutral Plasmas

Require external fields to mimic neutralizing background, or else Coulomb explosion would occur.

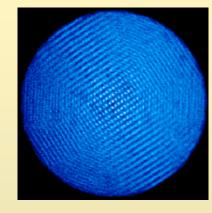




Paul Trap



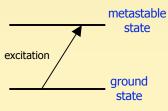
Penning Trap



3D Coulomb crystal ("Wigner" crystal)

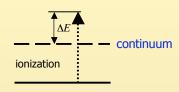
Neutral Plasmas

Require a trap to collect neutral atoms, but no plasma trap is needed.

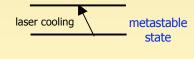


For example:

Xe τ =43s 6s[3/2]₂

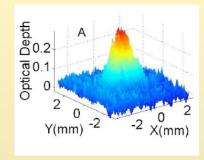


ground state



ground state

For example: $6p[5/2]_2 \\ N_{\chi e} \sim few 10^6 \\ n_{\chi e} < 10^{10} cm^{-3} \\ T_{\chi e} > 10 \mu K$



$$\Gamma_{ii} = e^2 / (a_{ic}T)_a = 2.7 \cdot 10^5 \left(n / 10^9 cm^{-3} \right)^{1/3} / (T / 10\mu K) \sim 300,000$$

$$\Gamma_{ee} = e^2 / \left(a_{ic} \frac{2}{3} \Delta E \right) \sim \Gamma_{ei} \sim 30$$



Dusty Plasmas

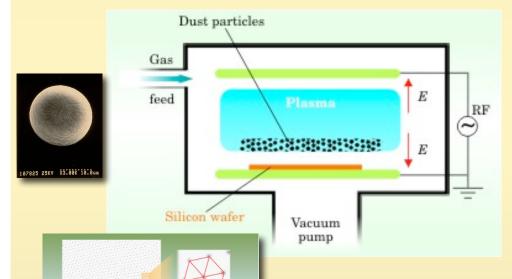
A dusty plasma is a "normal" plasma with is laced with macroscopic (micron-scale) grains (the "dust"). A sheath forms around each grain and a net negative charge results on the surface. The charge is roughly:

$$Qe \approx -2000 r_{grain} [\mu m] T_e [eV]$$

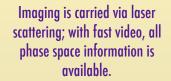
When it was realized that grains could have enormous charges, traps were designed and dust was manufactured.

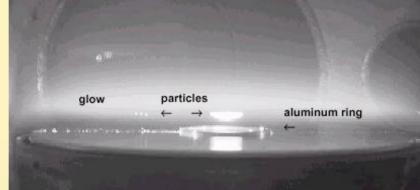


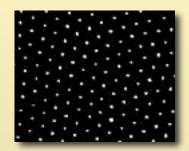
Dust fills the universe.



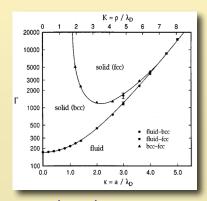
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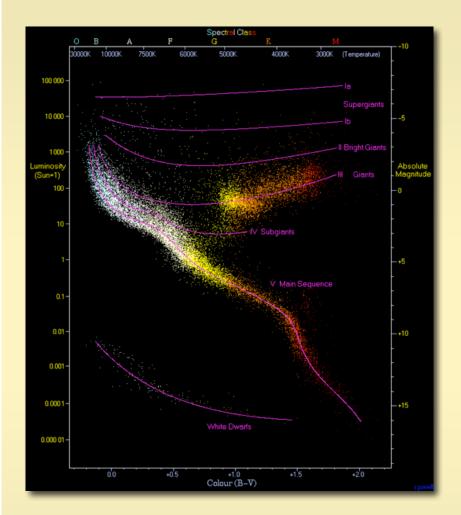
A 2D, classical "Wigner crystal"

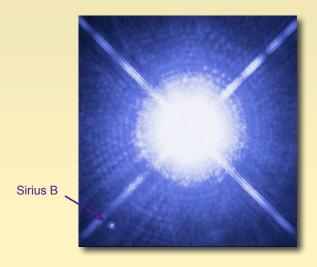


Yukawa Phase Diagram

LA-UR-08-0111

White Dwarfs





White Dwarf Facts:

- late stage of stellar evolution
- no longer burning fuel mainly C/O mixture
- collapse avoided by electron degeneracy
- very dense $\rho \sim 10^{7-10} \, \text{g/cm}^3$
- hot to warm $T \sim 10^{6-8} \text{ K}$
- cooling curves used as cosmochronometer

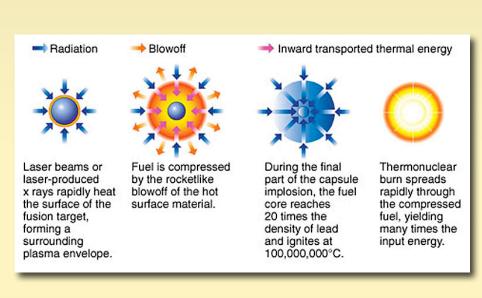
The electrons and ions in a WD have interesting properties:

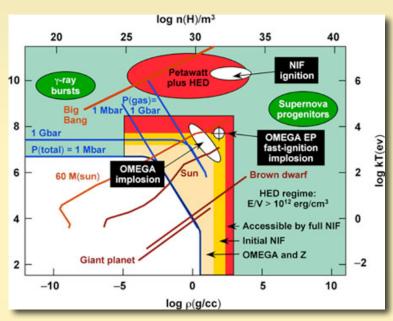
- electrons are very degenerate; they can be treated as a T=0 electron gas
- the Fermi is so high (~m_ec²) that the electrons are relativistic (~OCP model)
- the range of Coulomb coupling parameters for the ions is Γ ~10-1000
- core densities can be so high that the ions are mildly quantal



Inertial Confinement Fusion

One of the two major efforts toward controlled fusion energy is "inertial fusion," which utilizes high density and highly transient conditions.

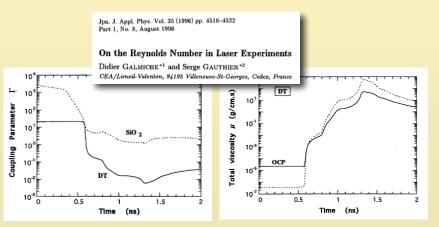




ICF is made possible by very large, usually laser, drivers:

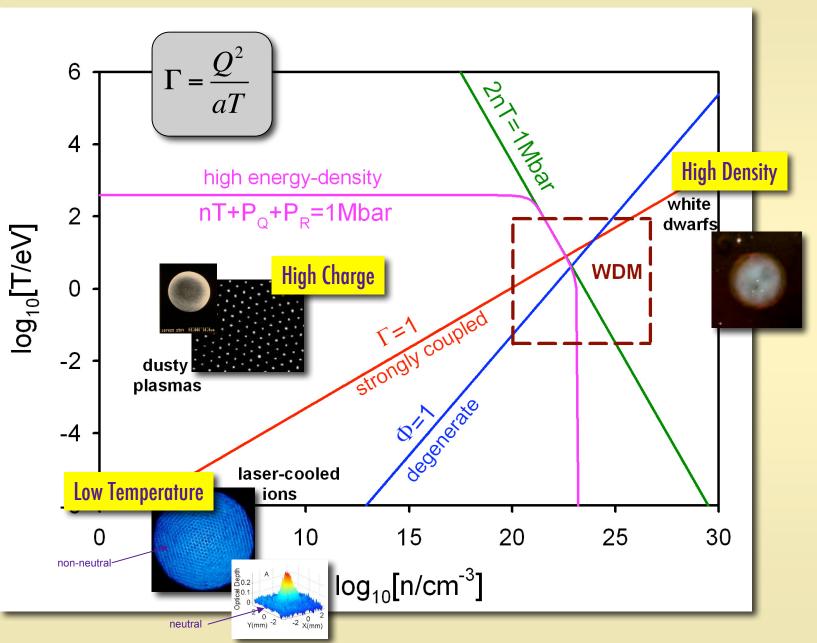
- NIF at LLNL
- Omega at Univ. of Rochester
- Z-machine at SNL
- HIF at LBNL
- Etc.

ICF experiments are strongly coupled at early times.





Summary of Examples of Strongly Coupled Plasmas





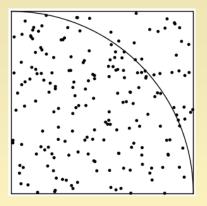
Monte Carlo Methods

We wish to compute such multidimensional integrals *exactly*.

$$Z = \frac{1}{\Omega^{N}} \int d^{3N} r e^{-U/T}$$

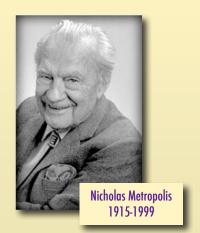
$$\langle A \rangle = \frac{\int d^{3N} r A(r^{3N}) e^{-U/T}}{\int d^{3N} r e^{-U/T}}$$

Multidimensional integrals can be done with random numbers.



area under curve= number of dots below curve area inside box

These integrals are very difficult to compute using Monte Carlo integration methods, because it is not known a priori where the important parts of the integral are.



Think of integration as a sampling of the phase space with a given probability of visiting various points.

$$\langle A \rangle = \frac{\int d^{3N} r A(r^{3N}) e^{-U/T}}{\int d^{3N} r e^{-U/T}}$$

$$= \int d^{3N} r A(r^{3N}) \left[\frac{e^{-U/T}}{\int d^{3N} r e^{-U/T}} \right]$$

$$= \int d^{3N} r A(r^{3N}) P(r^{3N})$$

$$= \int d^{3N} r A(r^{3N}) P(r^{3N})$$

$$\langle A \rangle \approx \frac{1}{M} \sum_{i=1}^{M} p_i A_i$$
Algorithm:

1. Select random particle
2. Compute U
3. Displace particle random
4. Compute U'; $\Delta U = U' - U$
5. If Prob=exp($\Delta U/T$)<1,

This problem is solved using the "Metropolis algorithm".

Algorithm:

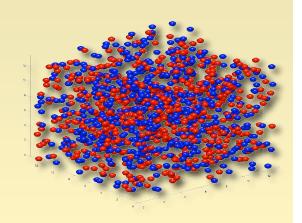
- 3. Displace particle randomly
- 4. Compute U'; $\Delta U=U'-U$
- 5. If Prob=exp($\Delta U/T$)<1, accept with Prob
- 6. Repeat



Molecular Dynamics: Most Versatile Method For SCPs

Molecular dynamics is based on:

- We assume we know the forces (Hamiltonian equations)
- The coupled equations-of-motion are integrated
- The full phase-space trajectory $\{r^{N}(t), p^{N}(t)\}\$ is computed/stored
- "Observables" are obtained from phase-space information



Molecular dynamics is exact, except:

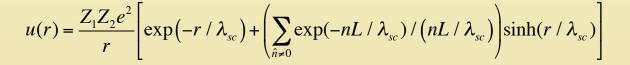
- finite timestep
- finite particle number
- boundary conditions
- finite statistics (length of run)
- forces may not be known
- poor convergence at high temperatures
- etc.

Detail for Coulomb Systems:

- Coulomb potential is long-ranged
- standard method to sum over infinite, periodic images used ("Ewald sum")
- spherical version used

What is done:

- monitor energy convergence
- simulate at progressively larger N
- usually "ignored"
- convergence examined
- do the best you can
- apply to SCPs, or develop alternate methods
- etc.





Integral Equations - Hypernetted Chain Approximation and Beyond

Recall that the MFT solution was a non-linear integral equation, which fails in the strong coupling regime - what to do?

Such integral equation methods are now well developed, and the HNC approximation is known to be best for long-range-potential problems.

Hypernetted Chain Approximation

$$h(r) = g(r) - 1$$

$$g(r) = \exp(-\beta u(r) + h(r) - c(r))$$

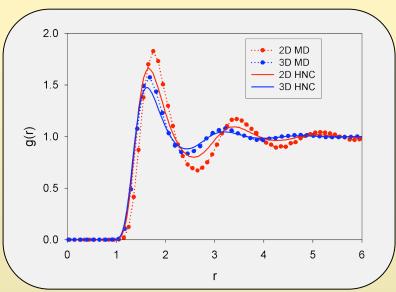
$$h(r) = c(r) + n \int dr' c(r')h(r - r')$$

We then easily get interesting information.

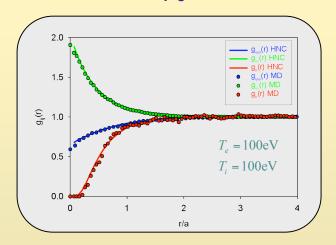
$$\frac{P}{nT} = 1 + \frac{\Gamma}{2} \int_{0}^{\infty} dr \, r \, h(r) e^{-\kappa r} (1 + \kappa r)$$

$$\frac{\partial P}{\partial nT} = 1 - 3 \int_{0}^{\infty} dr \, r^{2} \left[c(r) + \frac{\Gamma}{r} e^{-\kappa r} \right]$$
(shown here for Yukawa)

HNC very nearly captures exact solution.



HNC is easily generalized.

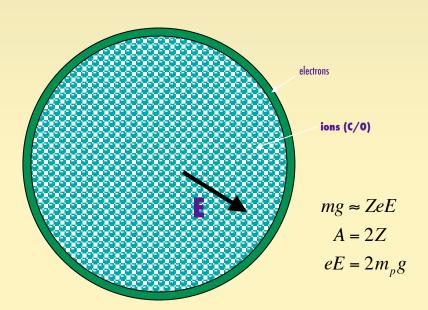


Dense hydrogen (electrons plus protons).



Sedimentation in White Dwarfs

Can impurities convert gravitational energy into heat, and thereby slow the cooling?



$$F_{down}^{22Ne}(r) = mg(r) - ZeE(r)$$

$$= 22m_p g - 10eE$$

$$= 22m_p g - 10\left(2m_p \frac{Gm(r)}{r^2}\right)$$

$$= 2m_p \frac{Gm(r)}{r^2}$$

Elements with a neutron excess will settle, and there is gravitational energy in ²²Ne to affect the overall energy content.

The drift velocity is related to the diffusion coefficient.

$$v = \mu F$$

$$= \left(\frac{D}{T}\right) \cdot \left(2m_p g\right)$$

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GRAVITATIONAL SETTLING OF ²²Ne IN LIQUID WHITE DWARF INTERIORS

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$$D^* = \frac{D}{\omega_p a^2}$$

$$\approx \frac{3}{\Gamma^{4/3}}$$

- ✓ Neglects screening
- ✓ Neglects physics of mixtures
- ✓ Neglects quantal effects



Transport Coefficients Obtained Via Kubo-Green Relations

Diffusion Coefficient: (velocity autocorrelation function)

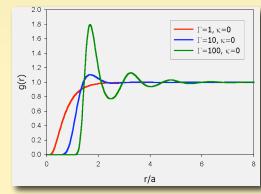
$$D = \int_{0}^{\infty} dt \left\langle v(t)v(0) \right\rangle$$

$$= \frac{T}{M} \int_{0}^{\infty} dt \, Z(t)$$

$$Z(t) = 1 - \Omega_{E}^{2} t^{2} + \cdots$$
Decay is not exponential.

$$\Omega_E^2 = \frac{4\pi n}{M} \int_0^\infty dr \, rg(r) \left[r \frac{d^2 u(r)}{dr^2} + 2 \frac{du(r)}{dr} \right]$$

Decay depends on pair correlation function.



Viscosity Coefficient: (stress-tensor autocorrelation function)

$$\eta = \frac{V}{T} \int_{0}^{\infty} dt \left\langle P_{\alpha\beta}(t) P_{\alpha\beta}(0) \right\rangle$$

$$P_{\alpha\beta} = \frac{1}{V} \left(\sum_{i} m_{i} v_{i\alpha} v_{i\beta} + \frac{1}{2} \sum_{i \neq i} r_{ij\alpha} f_{ij\beta} \right)$$

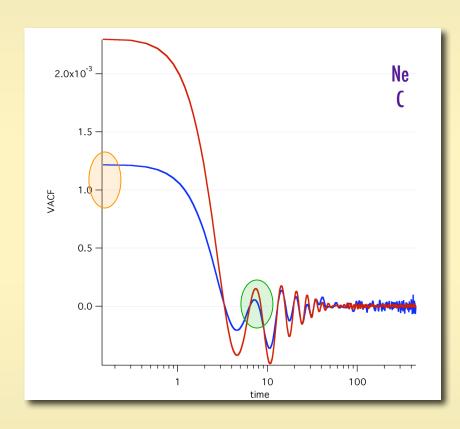


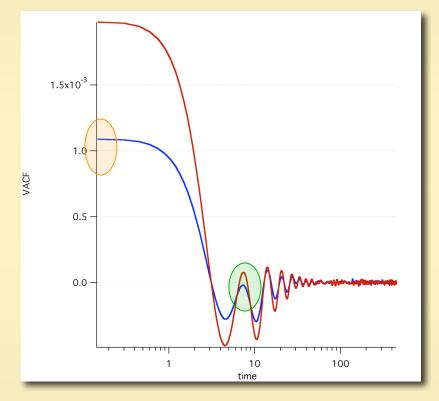
Typical Results for Ne Diffusion in Pure Carbon White Dwarf

Consider the case:

$$\Gamma = 150$$

$$\kappa = 0.312$$





$$x_{Ne} = 0.02$$

$$D^* = 0.0012$$

$$x_{Ne} = 0.25$$

$$D^* = 0.00045$$

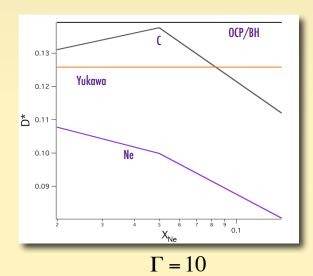


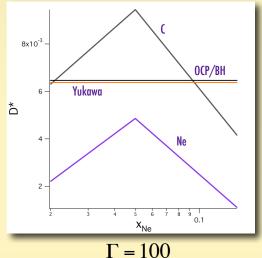
Comparison of Bildsten-Hall Model With Impurity Model

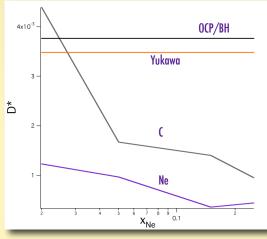
Effects of screening can be found by comparing OCP and Yukawa models:

Molecular dynamics evaluation of self-diffusion in Yukawa systems

artment of Fundamental Energy Science, Kyoto University, Gokasho, Uji, Kyoto 611-0011, Japan





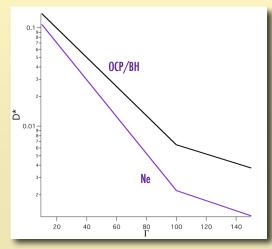


$$\Gamma = 100$$



Some basic conclusions:

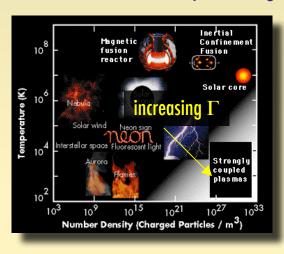
- Previous OCP and Yukawa results not fully converged.
- Screening is important at the \sim 20% level.
- Treating Ne as an impurity is important, and G-dependent.
- More, and better, results are needed.

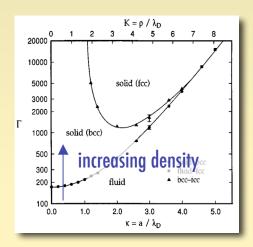


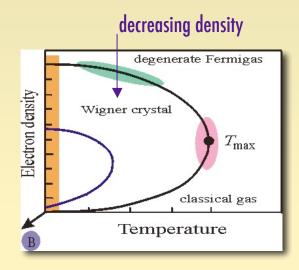


Warm Dense Matter - What Is It?

How can we reconcile these phase diagrams?







We cannot use the usual definition for electrons:

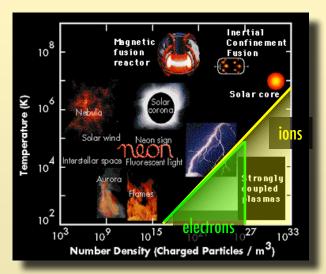
$$\Gamma = \frac{Q^2}{aT} = \frac{\langle \text{potential energy} \rangle}{\langle \text{kinetic energy} \rangle}$$

$$\Rightarrow \frac{Q^2}{a\sqrt{T^2 + E_F^2}}$$

$$E_F = \frac{\hbar^2 (3\pi^2 n)^{2/3}}{2m}$$

Very dense electrons are weakly coupled = easy!

This suggests defining a degeneracy parameter: $\Phi = \frac{T}{E_F}$



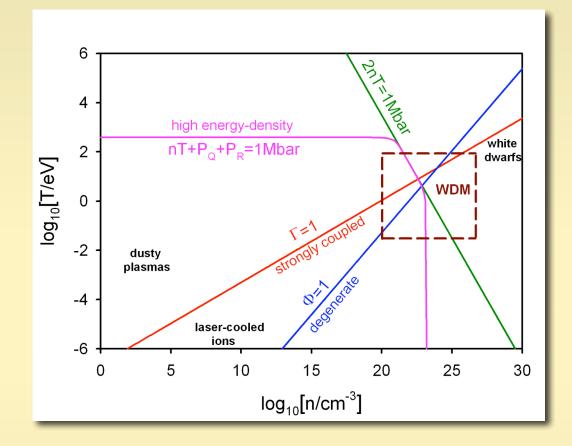
Warm Dense Matter - Where There Are No Expansion Parameters

From this perspective, we can define WDM as matter with:

$$\Phi \sim \frac{T}{E_F} \qquad \Gamma \sim 1$$

Not only can we not expand in these parameters, this definition also contains the conditions:

- temperature about ionization potential
- density about maximum packing of free atoms



Main Points:

- Warm Dense Matter is moderately coupled, enough so that MFT fails
- Warm Dense Matter is mildly degenerate such that quantum fluctuations compete with thermal fluctuations and reduce the effective coupling
- Warm Dense Matter is only *moderately* ionized

WDM = strongly coupled ions + moderately coupled electrons + dense atomic physics

- Warm Dense Matter is partially pressure ionized
- The WDM problem: All of these are true simultaneously!



A Warm Dense Matter Parameter

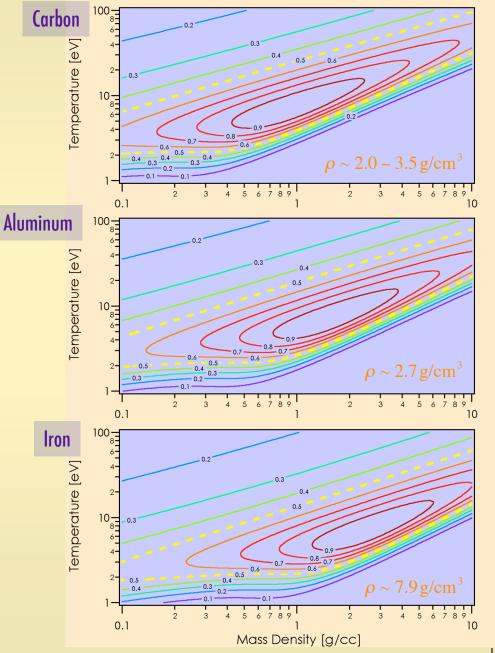
We can define a "WDM parameter" as:

$$W = \exp\left[-\left(1-\Gamma\right)^{2}\right] \cdot \exp\left[-\left(1-\Phi\right)^{2}\right]$$

For a real material, we need to consider ionization.

$$\begin{split} \overline{Z}(\rho,T) \\ n_e^f &= \overline{Z}(\rho,T) \frac{\rho}{M_i} \\ E_F &= \frac{\hbar^2 \left(3\pi^2 n_e^f\right)^{2/3}}{2m_e} \\ \Gamma_{ee} &= \frac{e^2}{a_e \sqrt{T^2 + E_F^2}} \end{split}$$

To estimate W, use a simple Thomas-Fermi model for $Z(\rho,T)$.





Summary

- The issue of strong coupling was introduced in the context of the simplest, nontrivial case the Ising Model
- Because perturbation theory isn't useful, mean field theory (MFT) was employed to illustrate basic issues
- extended to continuous systems, MFT yields the Poisson-Boltzmann equation for Coulomb systems
- Issues with long-range interactions were discussed
- Strongly Coupled Plasmas are statistical systems with long-range interactions for which MFT fails
- Real examples of SCPs were discussed (electrons on He, dusty plasmas, ultracold plasmas, white dwarfs)
- The three basic theoretical methods (MC, MD, integral equations) were described
- The example of sedimentation in white dwarfs, using MD, was shown
- The extension to quantum systems, and the connect to Wigner crystallization was described
- Finally, Warm Dense Matter was introduced as a type of SCP that is particularly complicated

